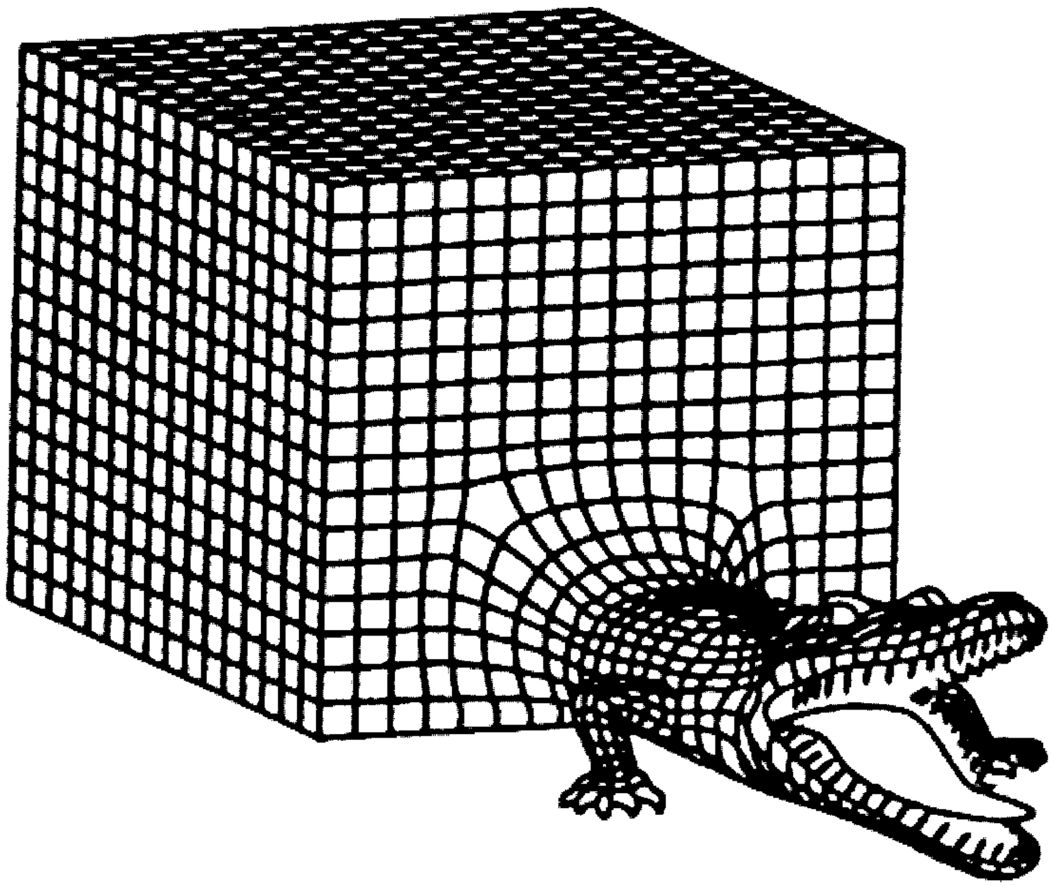
Dynamical Fermion Simulations: A Critical Status Report

Karl Jansen

- **Lattice actions**
  (an over-critical account)
- **Performance comparison**
- **Systematics**
  - continuum limit scaling
  - finite size effects
  - chiral perturbation theory
  - renormalization
  - effects of strange quark
  - mixed action
- **Conclusion**

Welcome to the lattice and its dangerous animals



Bem-vindos ‘a rede e seus animals perigosos

Добро пожаловать в теорию калибровочных полей на решётках... И в мир её опасных животных!

Bienvenidos a la Red y sus peligrosos animales

Dobrodosli na rešetku i opasne životinje na njoj

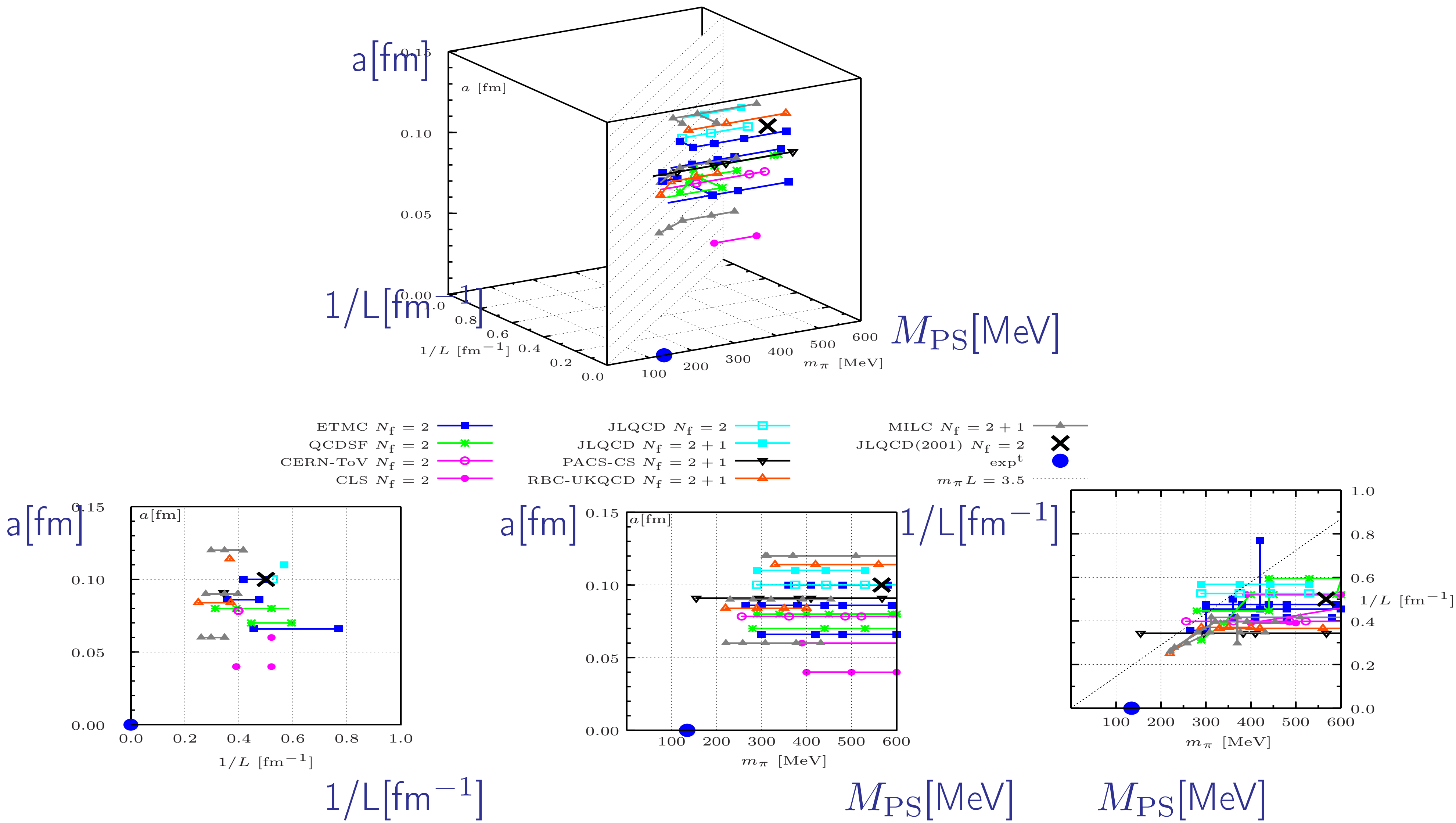
Willkommen auf dem Gitter und seinen gefährlichen Tieren

欢迎进入格点，
动物凶猛！

Witajcie na sieci, gdzie żyją niebezpieczne zwierzęta

Καλώς ήρϑατε στο πλέγμα και τα άγρια ϑηρία του

The parameter landscape (thanks to G. Herdoiza)



Non-perturbatively improved Wilson Fermions

This is most probably the best formulation of lattice QCD!

DRAWBACK

- for full non-perturbative $O(a)$-improvement

  $\longrightarrow$ **nonperturbative operator improvement neccessary**
  $\longrightarrow$ **very demanding (e.g. PDFs, formfactors etc.)**
  $\longrightarrow$ **sometimes neglected**

- **mixing under renormalization**

- **Moderate smearing can be helpful**
  does it harm?

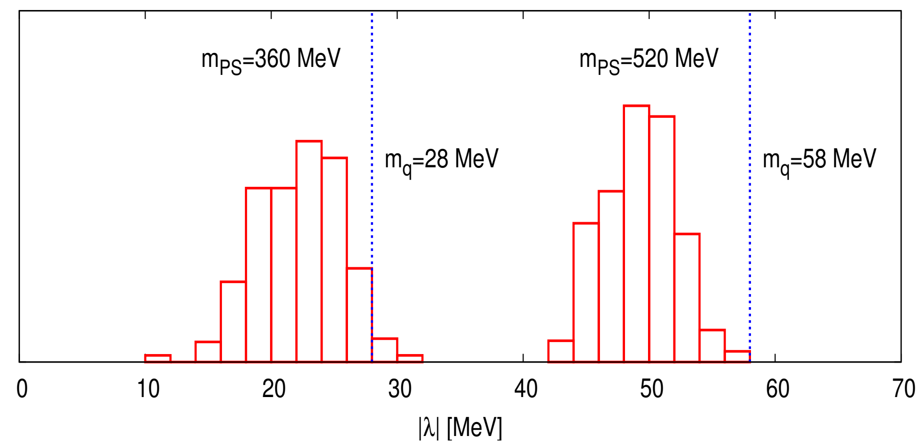
- **No infrared regulating quark mass**

Non-perturbatively improved Wilson Fermions

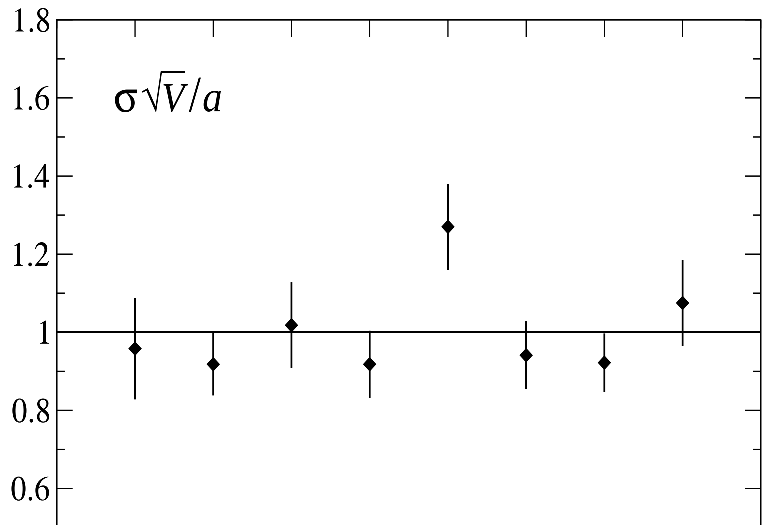
- No infrared regulating quark mass

  however

  stability through
  spectral gap
  (CERN)



smallest eigenvalue distribution with median $\bar{\mu}$ and width σ



median of distribution $\bar{\mu} \approx Zm$

demanding $\bar{\mu} \geq 3\sigma$

$\rightarrow m \geq 3a/Z\sqrt{V}$

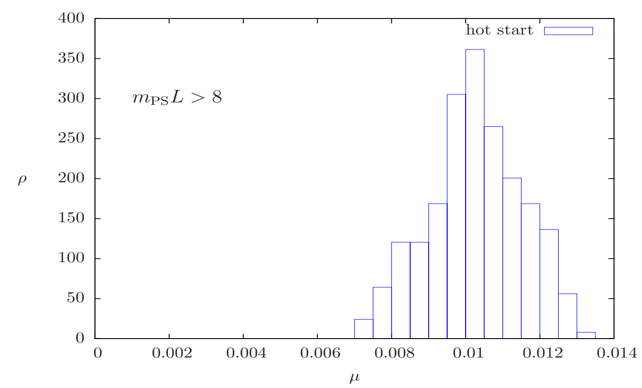
$\rightarrow m_\pi L \geq \sqrt{3\sqrt{2}aB/Z}$

Stability and Meta-Stability

(C. Urbach, K.J.)

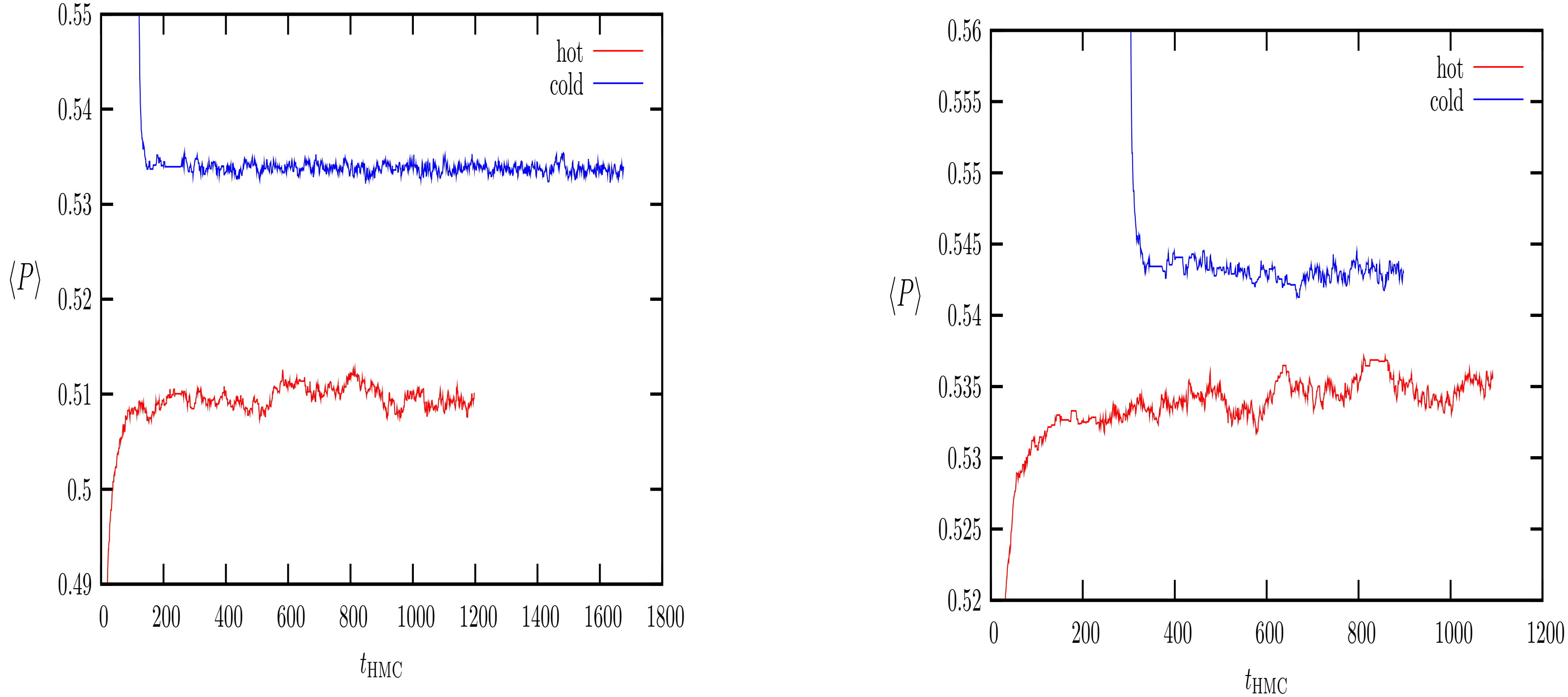
Wilson plaquette gauge action and Wilson fermion action

β	L	$m_{\mathrm{PS}}L$	$\bar{\mu}$	σ
5.2	16	8	0.0103	0.0013
5.3	16	4	0.0038	0.0010



$\Rightarrow$ all criteria fullfilled

Stability and Meta-Stability



→ different (hot and cold) starts

→ long-living metastable states at $\beta = 5.2$ and $\beta = 5.3$

→ check for metastable behaviour towards the chiral limit

(Sharpe, Wu; Münster, Hofmann; Scorzato; Farchioni et.al.)

rooted staggered fermions

This is most probably the best formulation of lattice QCD!

DRAWBACK

- **rooting issue still being discussed**
  - non-local at $a > 0 \Rightarrow$ scaling law towards continuum limit?
  - theoretical analysis **(Shamir; Sharpe; Bernard, Golterman, Shamir, Sharpe; Adams)**
  - non-perturbative couplings of tastes **(Creutz)**

- usage of non-exact RHMD algorithm
  - used for large volume simulations
  - no effect on plaquette **(Toussaint)** difference: $O(10^{-7})$
    (is it safe? what about e.g. correlators?)
  - exact RHMC algorithm about factor of 2 more expensive **(Gottlieb, Toussaint)**

rooted staggered fermions: two points of view

view I

- **First continuum limit, then chiral limit**
- **needs minimal pion mass**
  - continuum ChPT: taste splitting $\ll M_{\rm PS}^2$
  - staggered ChPT: taste splitting $\lesssim M_{\rm PS}^2$

    $a = 0.060$fm: $M_{\rm PS}^2 = (\approx 220{\rm MeV})^2 \approx 3*$ taste splitting

    $a = 0.125$fm: $M_{\rm PS}^2 = (\approx 250{\rm MeV})^2 \approx$ taste splitting

- Symanzik-like analysis **(Bernard, Golterman, Shamir)**

  $D_{\rm taste} = D_{\rm inv} + \Delta$ bound: $\|D_{\rm inv}^{-1}\Delta\| \lesssim a/(\underbrace{ma_c^2}_{\rm blocked})$

  $\Rightarrow$ continuum limit first

- **Order of limits: studied in Schwingermodel:**
  (Dürr, Hoelbling)

strategy seems to be working for all practical purposes
$\longrightarrow$ visit MILC presentations

rooted staggered fermions: two points of view

view II

- **Explore the chiral limit at fixed lattice spacing**
  in the end we are theorists ...

- check 't Hooft vertex **(Creutz)**
  (more general: observables related to instanton physics)

- explore ϵ-regime with simulations and chiral perturbation theory

maximally twisted mass fermions

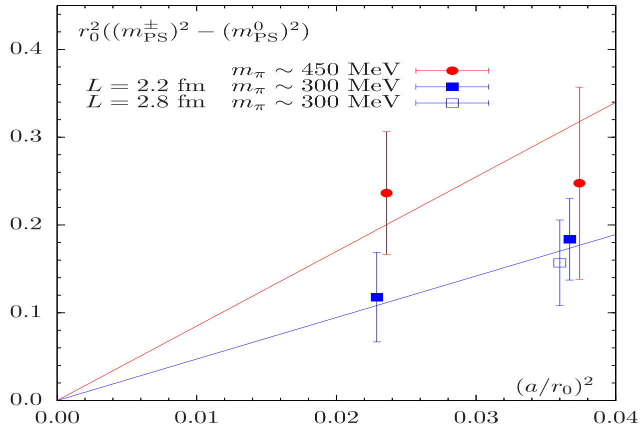
This is most probably the best formulation of lattice QCD!

DRAWBACK

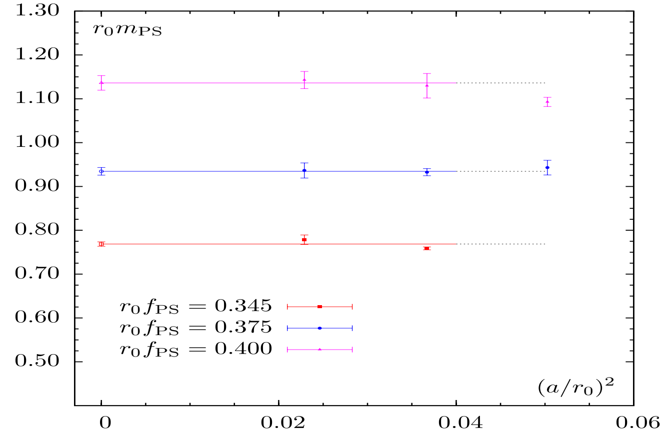
- neutral pion becomes zero at $\mu_{\rm tm} = \mu_{\rm tm}^{\rm crit}$
- isospin breaking

observation I

charged minus neutral



only charged



$\longrightarrow$ large cutoff effects in neutral pion mass

maximally twisted mass fermions

Observation II

$$R_O = \frac{O^{\pm} - O^0}{O^{\pm}}$$

	β	$a\mu_q$	R_O
af_{PS}	3.90	0.004	0.04(06)
	4.05	0.003	−0.03(06)
am_{V}	3.90	0.004	0.02(07)
	4.05	0.003	−0.10(11)
af_{V}	3.90	0.004	−0.07(18)
	4.05	0.003	−0.31(29)
am_{Δ}	3.90	0.004	0.022(29)
	4.05	0.003	−0.004(45)

- Isospin splittings compatible with zero for other (so far) considered observables

maximally twisted mass fermions

interpretation

analysis a la Symanzik

$$(m_{\mathrm{PS}}^{0})^2 = m_\pi^2 + a^2\zeta_\pi^2 + \mathcal{O}(a^2 m_\pi^2, a^4)\,, \qquad \zeta_\pi \equiv \langle \pi^0 | \mathcal{L}_6 | \pi^0 \rangle|_{\mathrm{cont}}$$

$$(m_{\mathrm{PS}}^{\pm})^2 = m_\pi^2 \qquad\qquad + \mathcal{O}(a^2 m_\pi^2, a^4)$$

ζ_π has a large contribution:

$$\zeta_\pi^2/\Lambda_{\mathrm{QCD}}^4 \sim 25 \gg a^2\Lambda_{\mathrm{QCD}}^4$$

size of isospin violation needs case by case study

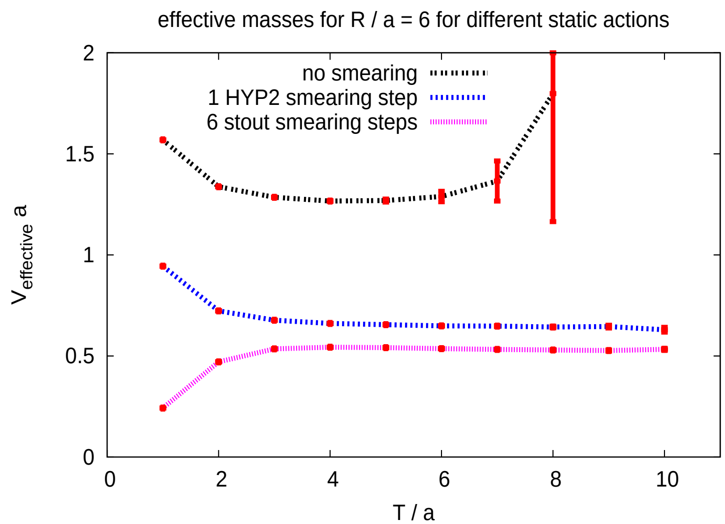
high (6) level stout smeared Wilson Fermions

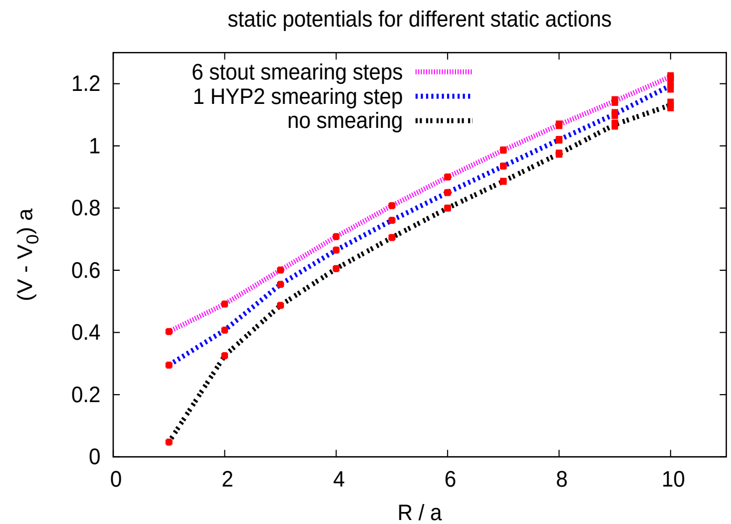
This is most probably the best formulation of lattice QCD!

DRAWBACK

- **alter short distance behaviour?**

→ here: look at static action **(Farchioni, Montvay, Urbach, Wagner, K.J.)**





$V_{\rm eff}$ **from below**   **no change at R/a relevant for r_0**

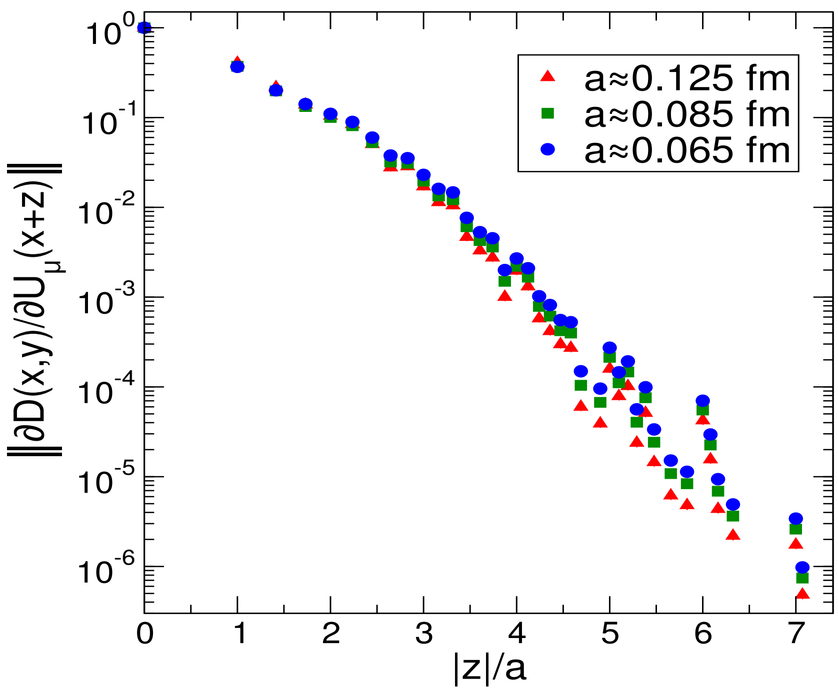
shift $r_0 \approx 6.0 \rightarrow r_0 \approx 4.8$ *why smaller?*

→ **compare lattice spacing from fermionic observable → in progress**

high (6) level stout smeared Wilson Fermions

- alter short distance behaviour?

→ check localization range of gauge field interaction



(BMW collaboration)

→ find exponential localization

Domain wall Fermions

This is most probably the best formulation of lattice QCD!

DRAWBACK

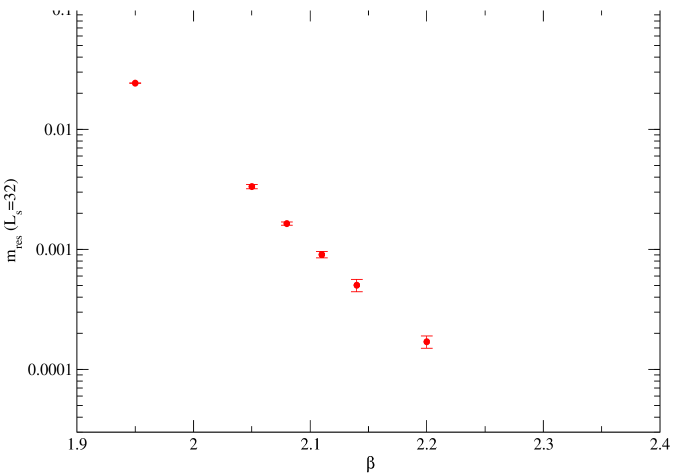
- Domain Wall Fermions with $N_S < \infty$ break chiral symmetry
  (as do imprecisely approximated overlap fermions)
  $\longleftarrow$ studied by RBC-UKQCD collaboration
- cost of improved chiral symmetry? $\longrightarrow$ later
- comparison $m_{\rm res}$ and $m_{\rm sea}^{\rm min}$

a^{-1}	$m_{\rm sea}^{\rm min}$	$m_{\rm val}^{\rm min}$	$m_{\rm res}$
1.73	0.005	0.001	0.00315(2)
2.42	0.004	0.002	0.000665(13)

Domain wall Fermions

- **Changing topology**

$m_{\mathrm{res}}(L_s)$ L_s fixed



β

- eigenvalue density of kernel operator

  $\rho(0) \longrightarrow 0$ for $\beta \longrightarrow \infty$

  $m_{\mathrm{res}} \propto \rho(0)/L_s$

  $\Rightarrow$ topology change forbidden for $a \longrightarrow 0$

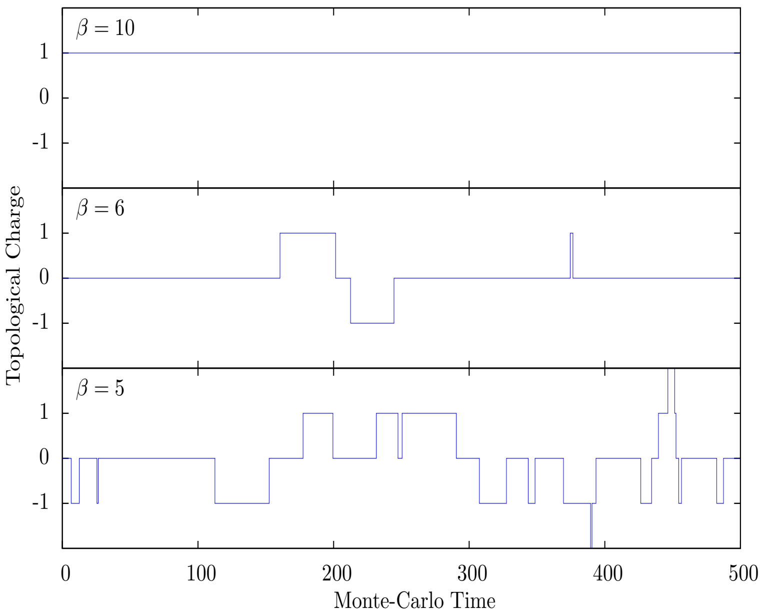
- consequence of negative quark mass plaquette bound

- holds true also for overlap fermions

Changing topology

what about other fermions?

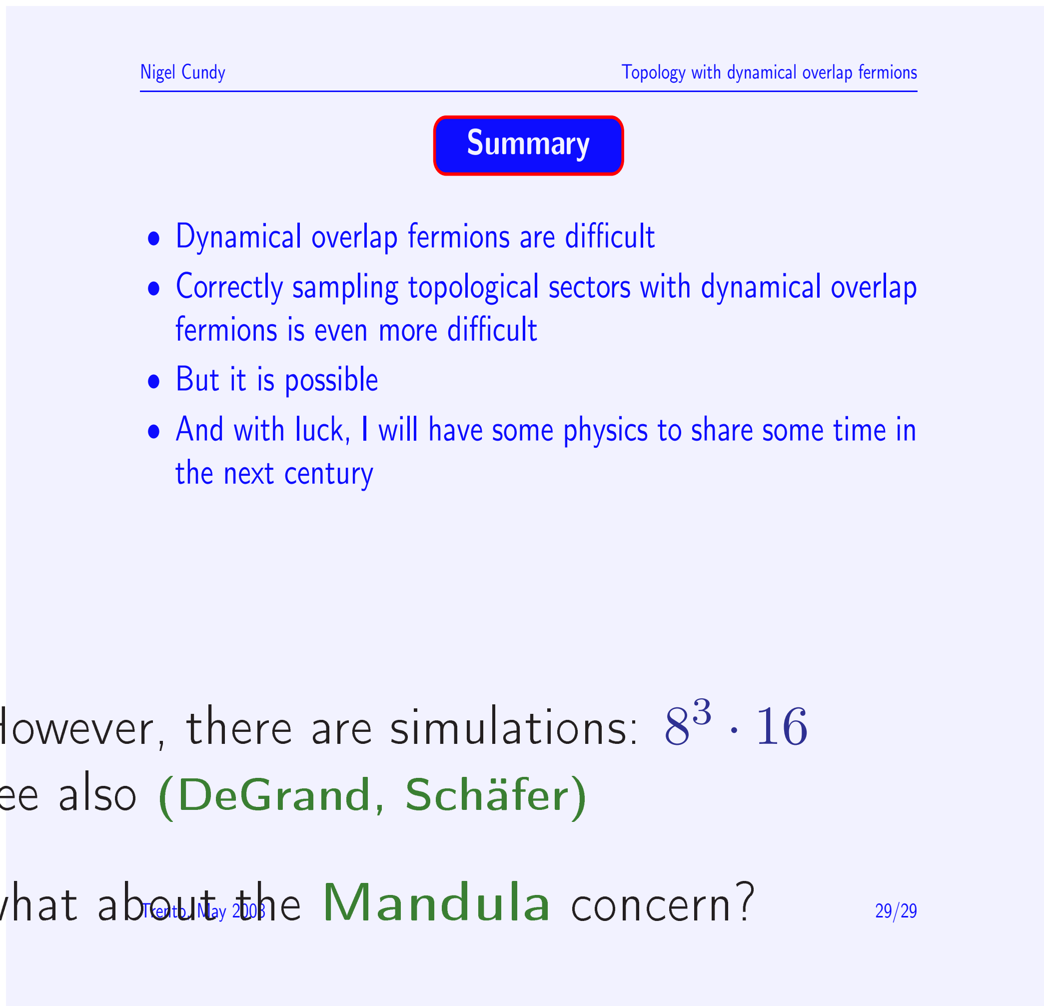
Schwinger model with Wilson fermions (Christian, K.J.)

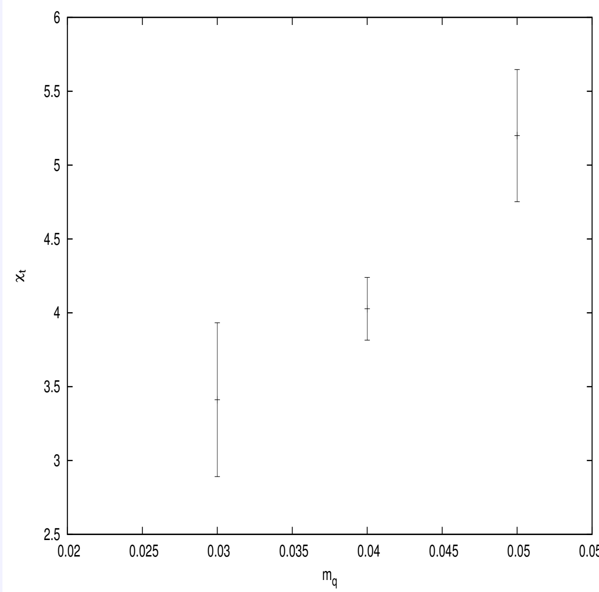


difficulty to change topology in principle problem for everybody
$\longrightarrow$ think about algorithms

overlap fermions

This is most probably the best formulation of lattice QCD!





χ_{top}

- However, there are simulations: $8^3 \cdot 16$
  see also **(DeGrand, Schäfer)**
- what about the **Mandula** concern?

overlap fermions in fixed topology

This is most probably the best formulation of lattice QCD!

- **effects of fixing topology**
  - topological finite size effects **(Brower et.al., Aoki et.al)**
  - algorithmic ergodocity
  - loss of clustering properties
- **worth the effort? $\longrightarrow$ main motivation: ϵ-regime**
  - fixed point action
    (P. Hasenfratz, Hierl, Maillart, Niedermayer, A. Schäfer, Weiermann, Weingart)
  - Wilson action **(A. Hasenfratz, Hoffman, S. Schäfer)**
  - twisted mass action **(Nube, Shindler, Urbach, Wenger, K.J.)**

  $\Leftarrow$ formulae in ChPT available summing over all topologies

- *Wilson determinant and O(a) effects?*
- $\tau_{\mathrm{int},N_{\mathrm{inv}}} \propto O(100)$; Q **independent?**
- continuum form of chiral Lagrangian but breaking of Lorentz invariance

Other Collaborations/Fermions

These are for sure ...

- Flic fermions (CSSM)
- Chirally improved fermions (BGR collaboration)
- Fixed point action (Bern group)
- Stout smeared Wilson (Hasenfratz, Hoffmann, Schäfer)

Disclaimer: *Don't forget, I have been over-critical here and played devil's advocate!*

In general, I think, we are doing very well

Cost of simulations

cost formula

$$C_{\mathrm{op}} = k \left(\frac{20\ \mathrm{MeV}}{\bar{m}}\right)^{c_m} \left(\frac{L}{3\ \mathrm{fm}}\right)^{c_L} \left(\frac{0.1\ \mathrm{fm}}{a}\right)^{c_a}\ \mathrm{Tflops} \times \mathrm{years}$$

$\bar{m}$ renormalized quark mass at 2GeV

(sorry for shoehorning you to this form ...)

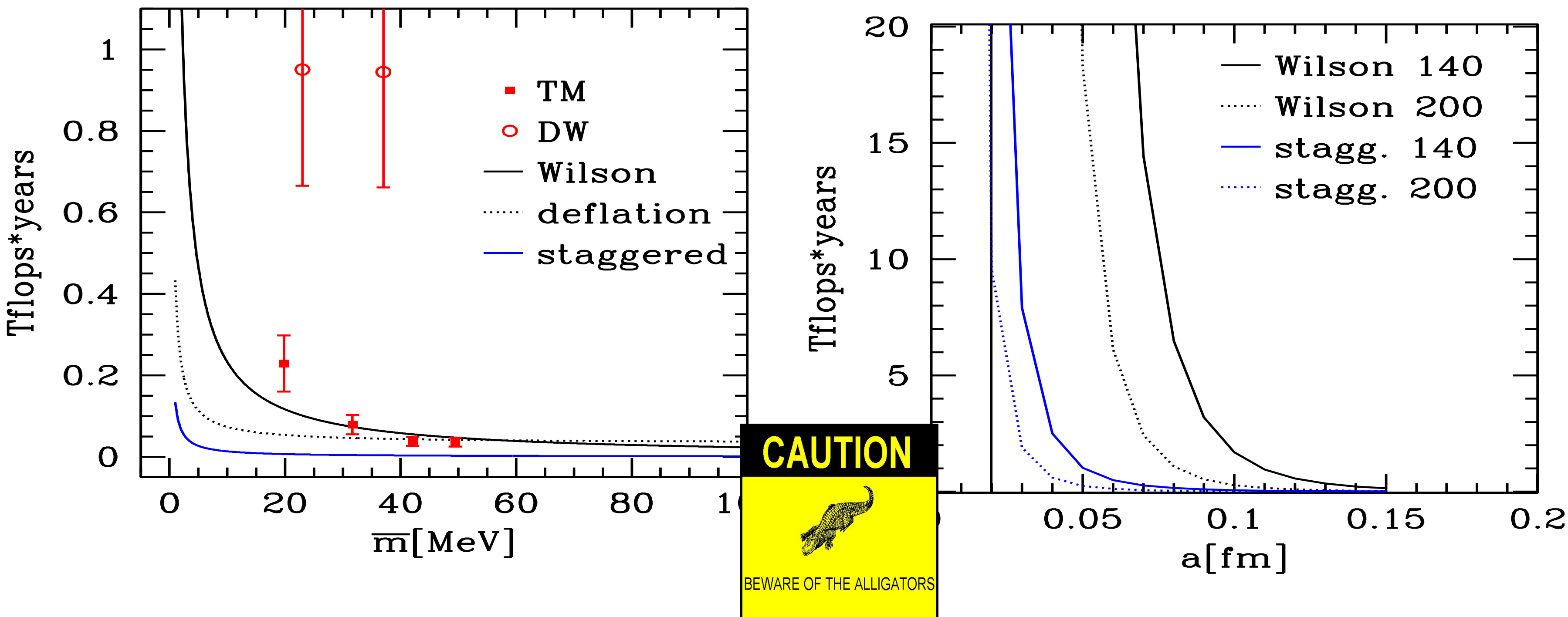
action	k	c_m	c_L	c_a
Wilson (DDHMC)	0.3	1	5	6
staggered (RHMC)	0.016	1	4	4
tmQCD (MTMHMC)	$0.8 - 2.1$	2	5	6

– $k,\ c_a,\ c_m,\ c_L$: large uncertainties

– not to be taken as definite

– e.g. c_a not confirmed by ETMC data
(scaling in a much weaker)

Updated Berlin Wall plot



$L = 2.1\text{fm}\ a = 0.087\text{fm}$,
1000 independent configurations

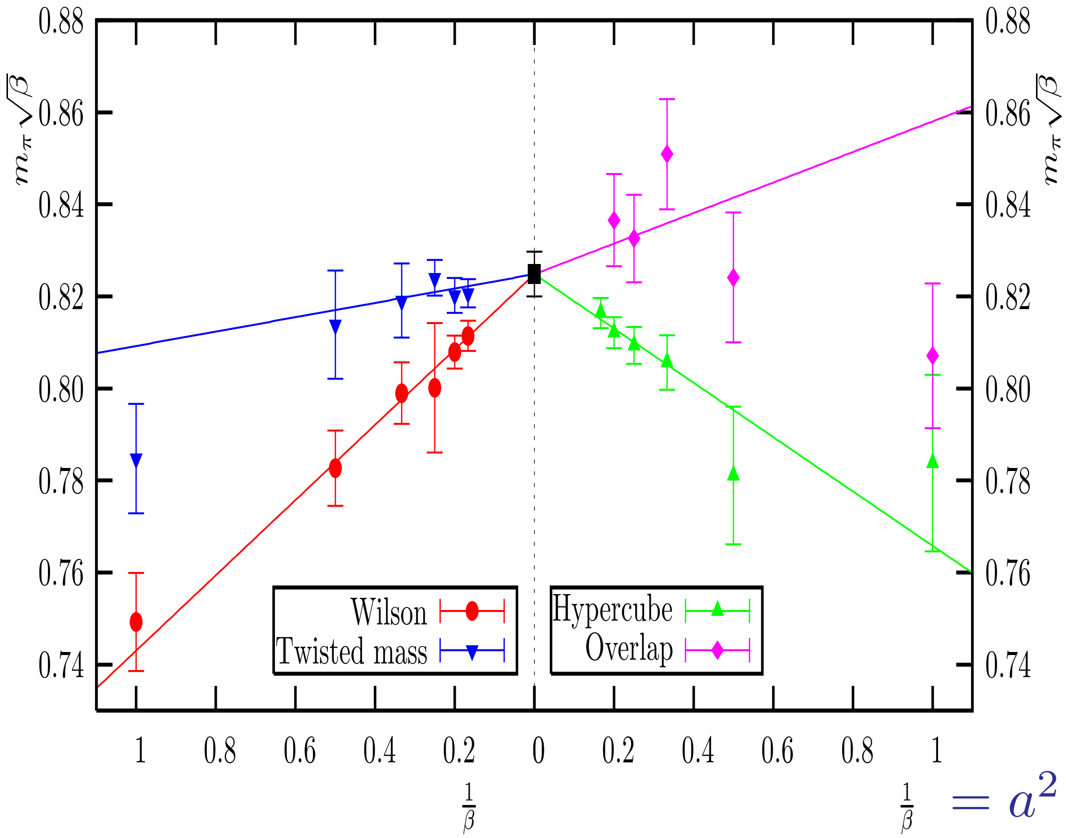
$M_{\rm PS}L = 3.5$

tremenduous algorithmic improvement
folded with machine capacities outperforming Moore's law
$\Rightarrow$ realistic simulations

It's universality

Example of the Schwinger model

(N. Christian, K. Nagai, B. Pollakowski, K.J.)



$\frac{1}{\beta} = a^2$

- $m_{\mathrm{quark}}\sqrt{\beta}$ fixed
- observe a^2 scaling
- universality of continuum limit
- $\approx 10\%$ scaling violation

Continuum limit scaling

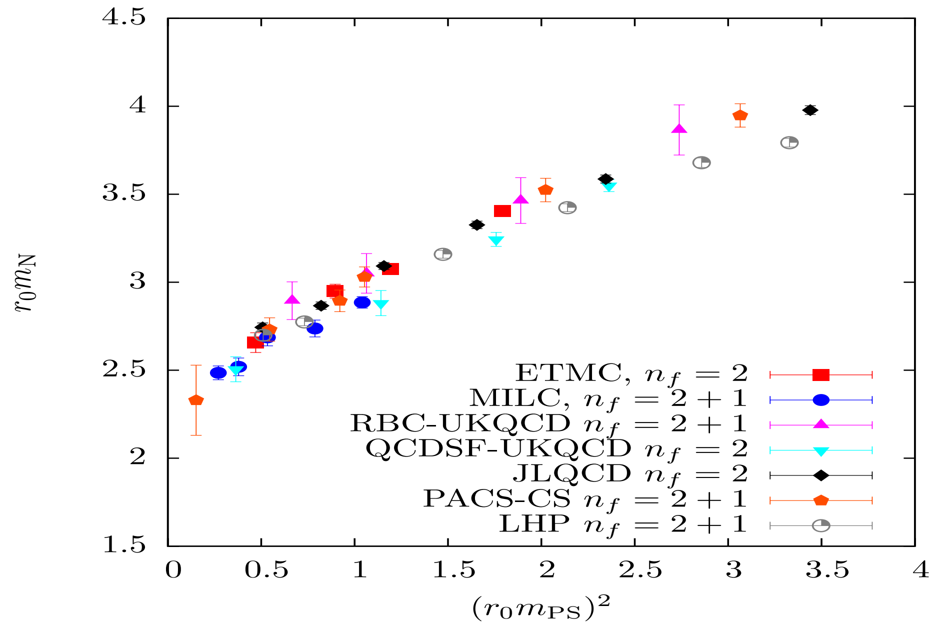
(Urbach, K.J.)

- use r_0 but
  - consider r_0 as scaling variable
  - not as physical quantity
- r_0 better than using the scale a^{-1}
- r_0 extrapolated to the physical point
- fix $r_0 M_{\rm PS} = 0.8, 1.0, 1.2$
- consider $r_0 f_{\rm PS}$ and $r_0 M_{\rm nucleon}$
- finite size corrections are taken into account $(f_{\rm PS}, M_{\rm PS})$

note: $f_{\rm PS}$ does not need renormalization for overlap, twisted mass and staggered fermions

Continuum limit scaling: nucleon mass

- the nucleon mass revisited



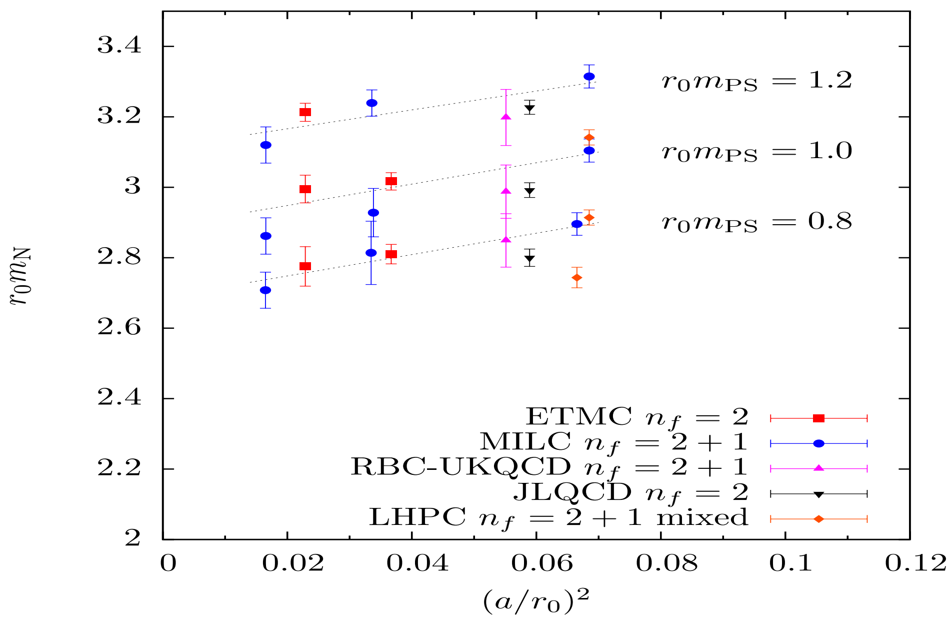
only smallest lattice spacing

$\longrightarrow$ no obvious discrepancy

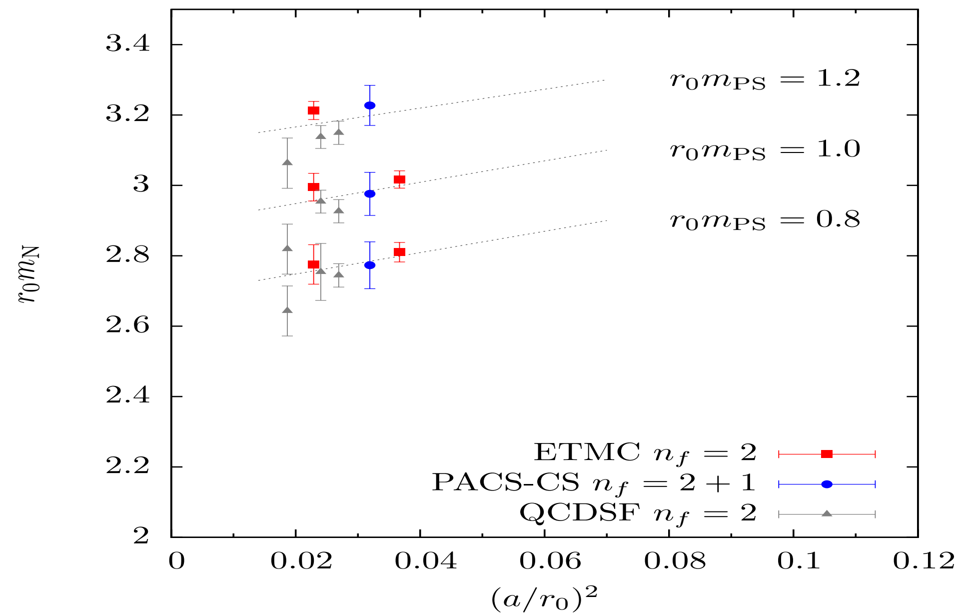
$\longrightarrow$ effects of scale setting

Continuum limit scaling: nucleon mass

staggered, DW, overlap



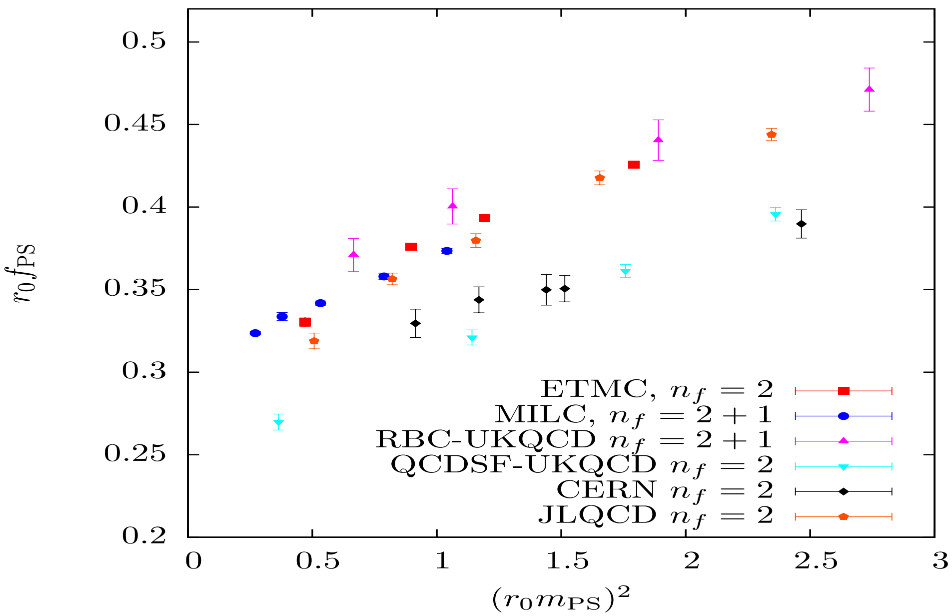
Wilson fermions only



$\longrightarrow$ find overall consistency

$\longrightarrow$ eventually combined continuum limit possible

Continuum limit scaling: f_{PS}

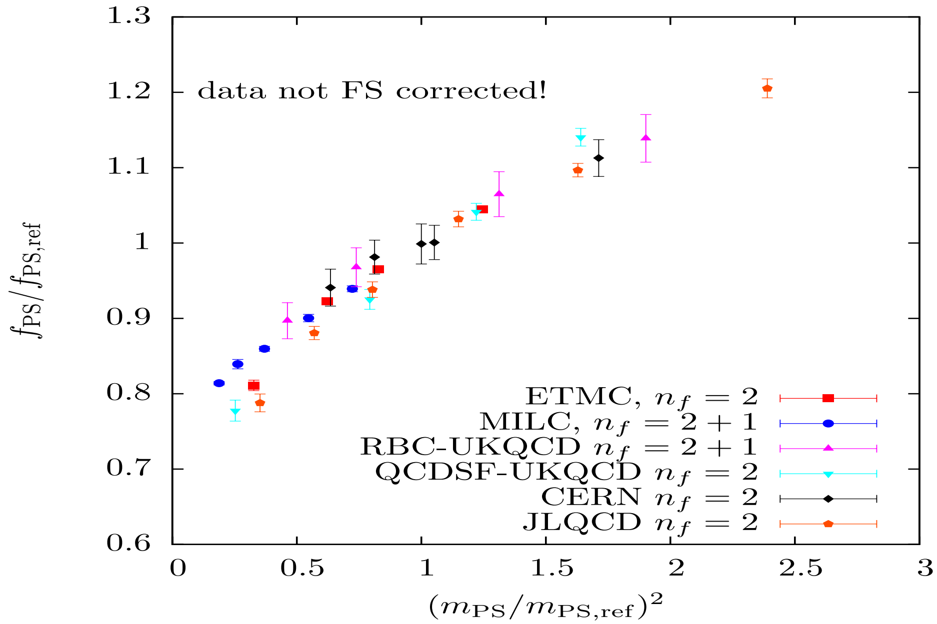


smallest lattice spacing only

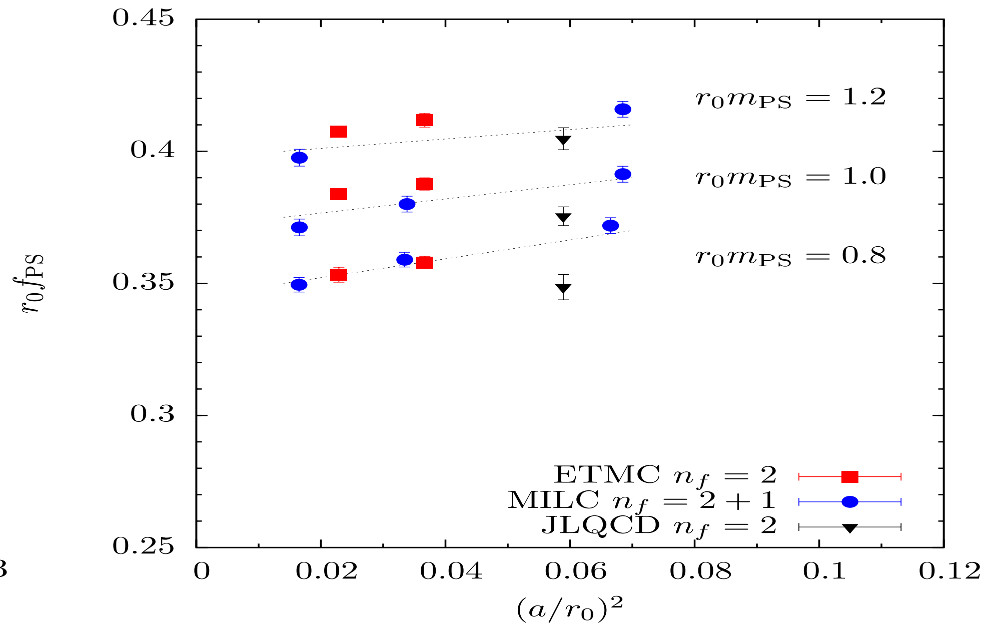
no signs of common scaling

Continuum limit scaling: $f_{\rm PS}$

$F_{\rm PS}$ normalized to reference point



only formulations with $Z_A = 1$



Continuum limit scaling: f_{PS}

possible sources of mismatch

- non-perturbative renormalization factor Z_A
- value for r_0
  varies from $r_0 = 0.45 - 0.5\mathrm{fm}$
  varies in time ...
- finite size effects
- N_f versus $N_f = 2 + 1$

$\Rightarrow$ need to understand this!

Do we need non-perturbative renormalization?

- strange quark mass **(tm-example, arXiv:0709.4574)**

$Z_P^{\mathrm{RI-MOM}}(1/a) = 0.39(1)(2)$ ← non-perturbative RI-MOM method

$Z_P^{\mathrm{BPT}}(1/a) \simeq 0.57(5)$ ← one-loop boosted perturbation theory

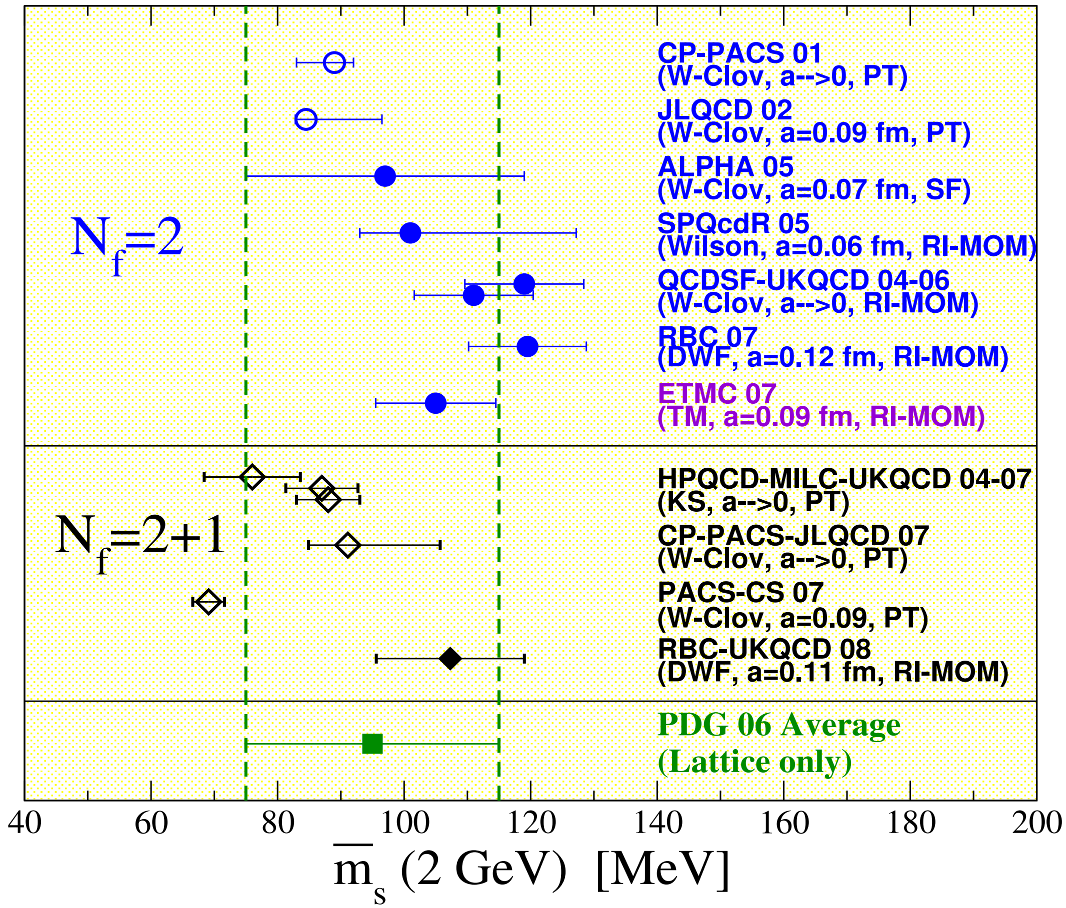
$m_q^{\overline{\mathrm{MS}}}(2\mathrm{GeV})\mathrm{MeV}$	perturbative	non-perturbative
m_{ud}	$2.63 \pm 0.08 \pm 0.36$	$3.85 \pm 0.12 \pm 0.4$
m_{ud} (PACS-CS)	2.53 ± 0.05	
m_s	$72 \pm 2 \pm 9$	$105 \pm 3 \pm 9$
m_s (PACS-CS)	72.7 ± 0.8	

Do we need non-perturbative renormalization?

- want massless renormalization scheme
  - $N_f = 2$
    RI-MOM: chiral extrapolation
    SF: direct at $m_{\mathrm{quark}} = 0$
  - $N_f = 2 + 1$
    RI-MOM: presently, only light quarks chirally extrapolated, strange fixed
    (RBC-UKQCD) **estimates systematic effects**
    SF: first simulations **(talk by Taniguchi)**
- renormalization needs dedicated runs with $N_f = 3$ mass degenerate quarks
- appetizer: this checks simultaneously SU(3) ChPT
  MILC is planning to perform such runs

Effects of dynamical strange?

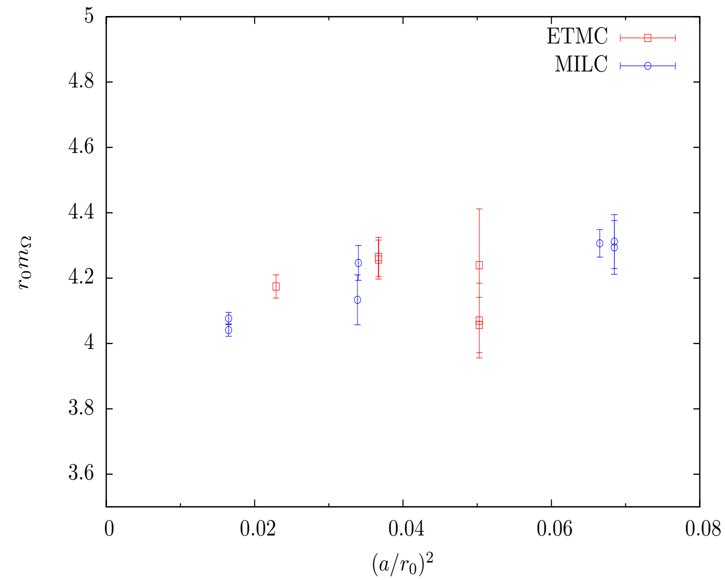
strange quark mass compilation (compiled by V. Lubicz)



→ no obvious effect of dynamical strange quark

Effects of dynamical strange?

take the $\Omega(sss - baryon)$-mass: chiral limit, no strong decay



- $r_0 M_{\rm PS}$ fixed

$\longrightarrow$ no obvious effect (however, large errors)

Mixed action

overlap on twisted mass sea: match $M_{\rm PS}$ (Garron, Scorzato)

$\longrightarrow$ find at matching point: $f_{\rm PS}(\rm tm) = 0.0646(4)$

$$f_{\rm PS}(\rm overlap) = 0.054(3)$$

domain wall on rooted staggered fermions: match $M_{\rm PS}$ (LHP collaboration)

$\longrightarrow$ find at matching point: $M_{\rm nucleon}(\rm staggered) = 0.723(6)$

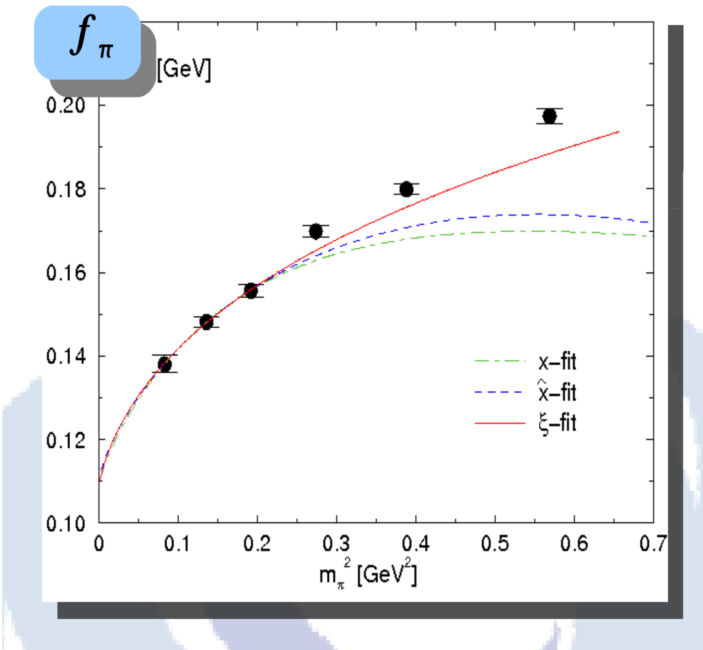
$$M_{\rm nucleon}(\rm domainwall) = 0.696(7)$$

check cutoff effects in mixed action calculations

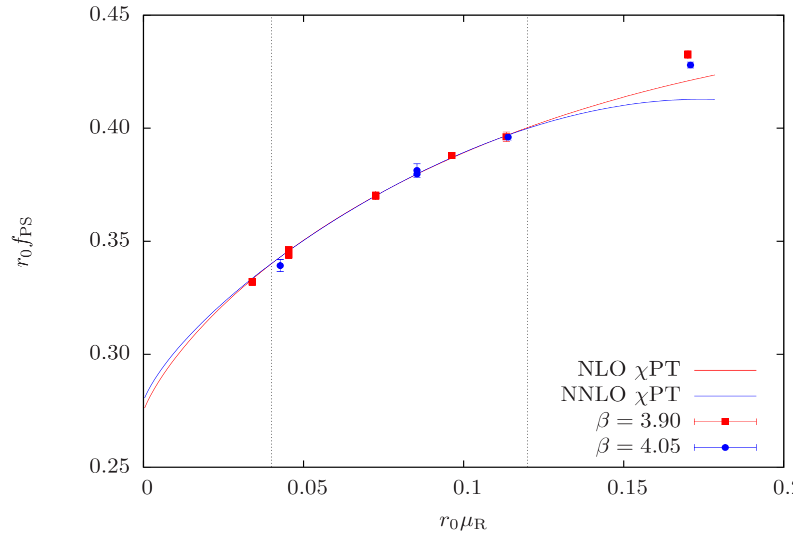
$\longrightarrow$ chiral perturbation theory analysis
(Bär, Rupak, Shoresh; Golterman, Izubuchi, Shamir)

where to apply 1-loop and 2-loop chiral perturbation theory?

- SU(2) χPT



(JLQCD)



(ETMC)

$$x = \frac{2B_0 m_q}{(4\pi f)^2}$$

$$\hat{x} = \left(\frac{m_\pi}{4\pi f}\right)^2$$

$$\xi = \left(\frac{m_\pi}{4\pi f_\pi}\right)^2$$

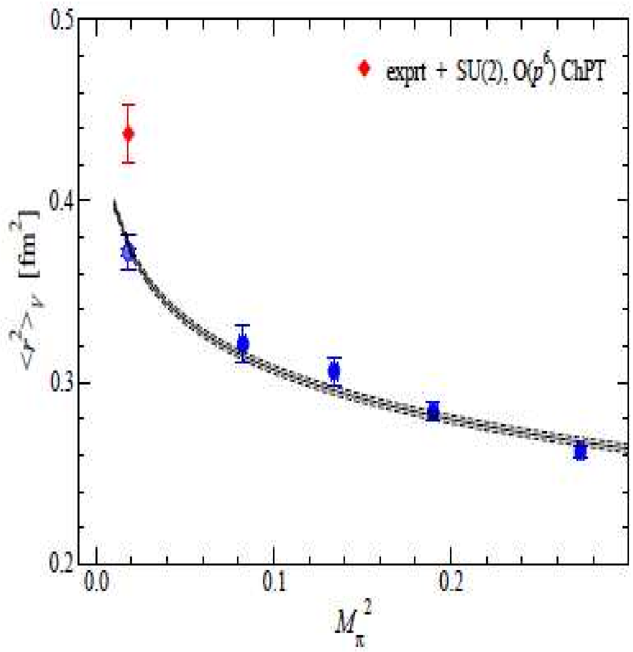
$$x = \frac{2B_0 m_q}{(4\pi f)^2}$$

finite size corrected

$\Rightarrow$ NLO for $M_{\rm PS} \lesssim 450$MeV valid (?)

NNLO needed?

scalar radius:



← JLQCD

$$\langle r^2 \rangle_V^\pi = \frac{1}{(4\pi f_\pi)^2}\left[\ln\frac{m_\pi^2}{\mu^2} + 12(4\pi^2)l_9\right]$$

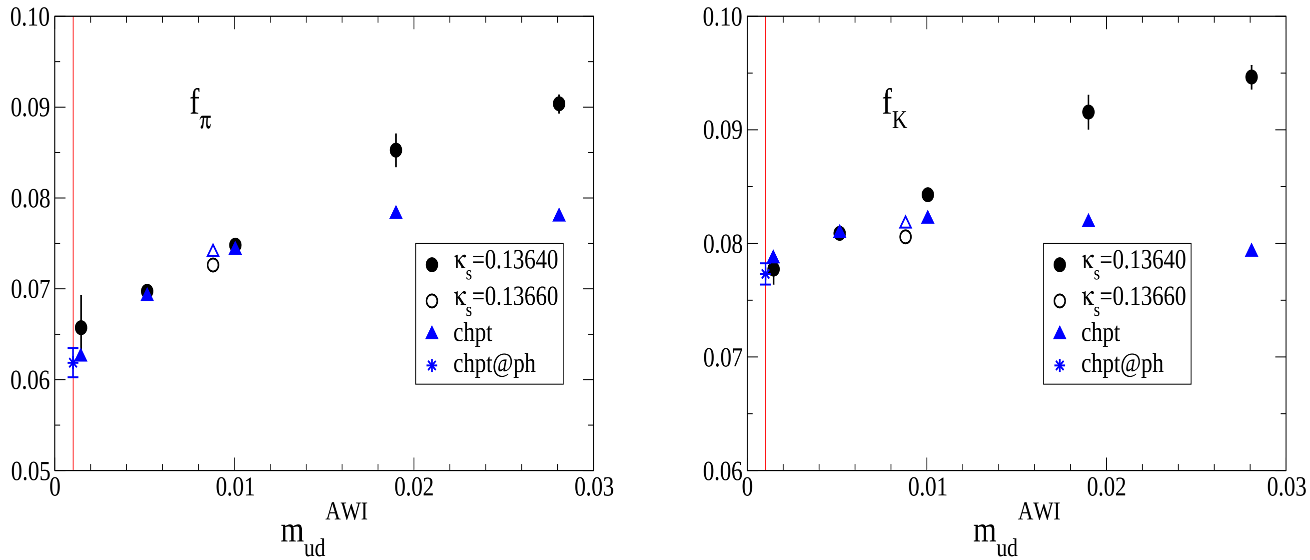
also seen by

ETMC

$$\langle r^2 \rangle_{\text{charge}}^\pi = \frac{1}{(4\pi f_\pi)^2}\left[\ln\frac{\Lambda_6^2}{2Bm} - 1\right]$$

$N_f = 2 + 1$ flavours

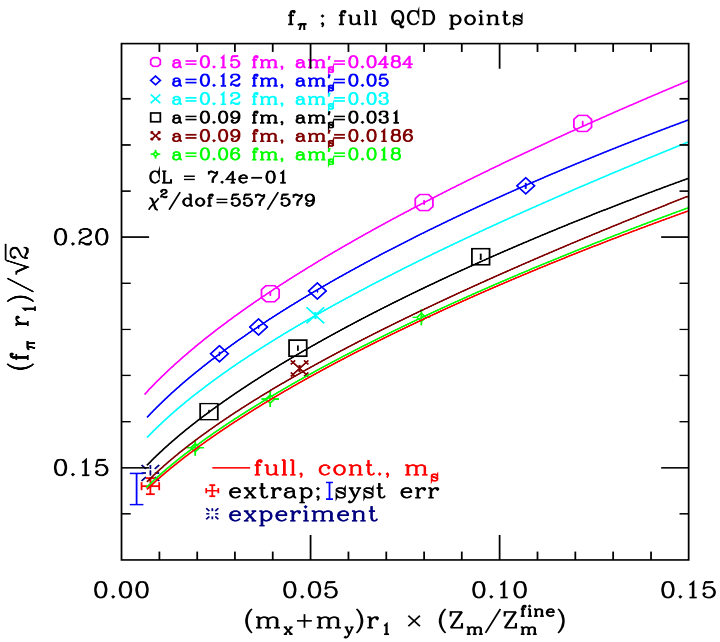
- SU(3) chiral perturbation theory
  example: **(PACS-CS)**



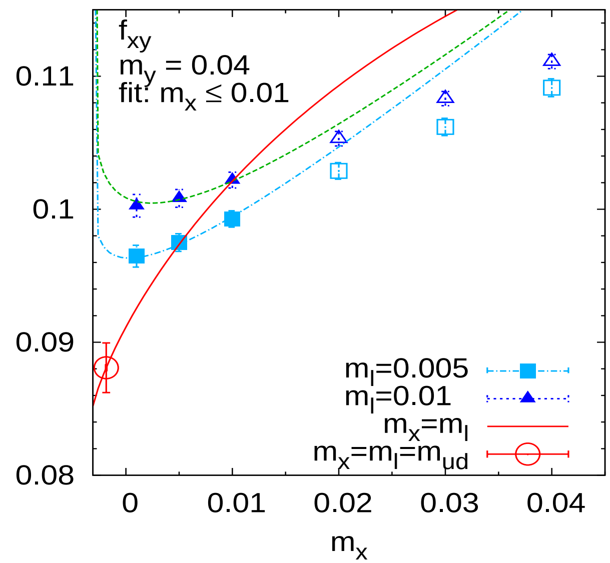
$\Rightarrow$ SU(3) not a good description
also concluded by other groups

$N_f = 2 + 1$ flavours

- SU(2) chiral perturbation theory
  - partially quenched chiral perturbation theory
  - fits work for $m_{\rm quark} \lesssim 0.01$ ($M_{\rm PS} \lesssim 450$ MeV)



(MILC)



(RBC-UKQCD)

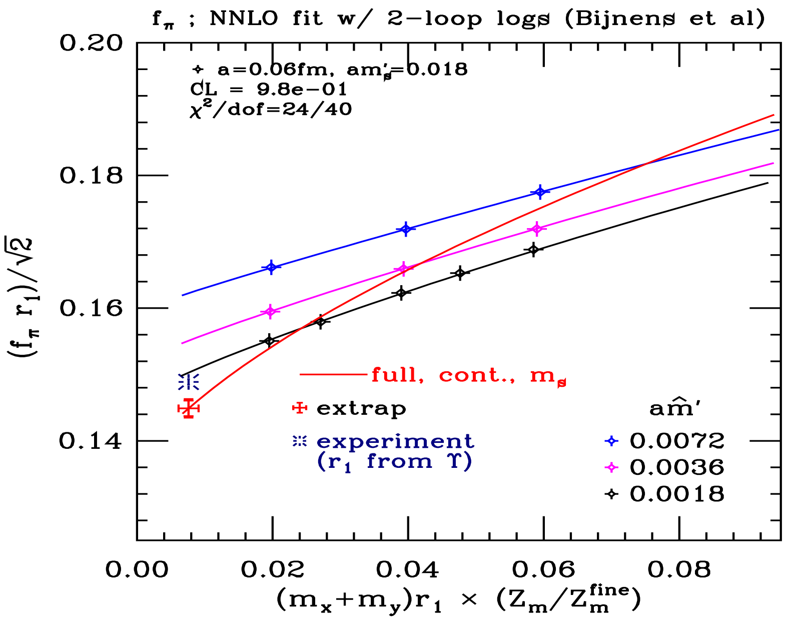
rooted staggered perturbation theory
add NNLO anayltic terms
(only sea quark data shown)

kaon ChPT
issue of uncorrelated fits

$N_f = 2+1$ flavours

staggered data at $a = 0.06$fm seem to be close to continuum $\Rightarrow$

- SU(2) 2-loop continuum chiral perturbation theory
  (rSχPT is not catching up to this order)
  $\longrightarrow$ extend fit range



(C. Bernard, MILC)

A comparison

	B	f	$\bar{l}_3$	$\bar{l}_4$
SU(2)×SU(2)	2.414(61)	0.0665(21)	3.13(33)	4.43(14)
SU(3)×SU(3)	2.457(78)	0.0661(18)	2.87(28)	4.10(05)
MILC $(N_f = 2+1)$			0.6(1.2)	3.9(5)
MILC, pure NLO			2.85(07)	–
ETMC $(N_f = 2)$			3.44(08)(35)	4.61(04)(11)
CERN $(N_f = 2)$			3.0(5)	–
phenom.			2.9(2.4)	4.4(0.2)

E. Scholz, RBC-UKQCD

Summary chiral perturbation theory

$N_f = 2$

- SU(2) χPT seems to work for $M_{\mathrm{PS}} \lesssim 450\mathrm{MeV}$
  - 2-loop effects seem to be important for pion radii
  - constraining fits, add more observables, go down to 200MeVpion masses

$N_f = 2 + 1$

- SU(3) χPT not working for kaon sector
  - to explore SU(3) χPT $\longrightarrow$ need $N_f = 3$ simulations (seems to be request from χPTheorists (Colangelo))
  - SU(2) χPT including lattice artefacts works for $M_{\mathrm{PS}} \lesssim 450\mathrm{MeV}$
  - continuum SU(2) χPT at NNLO

final check: χPT after continuum extrapolation

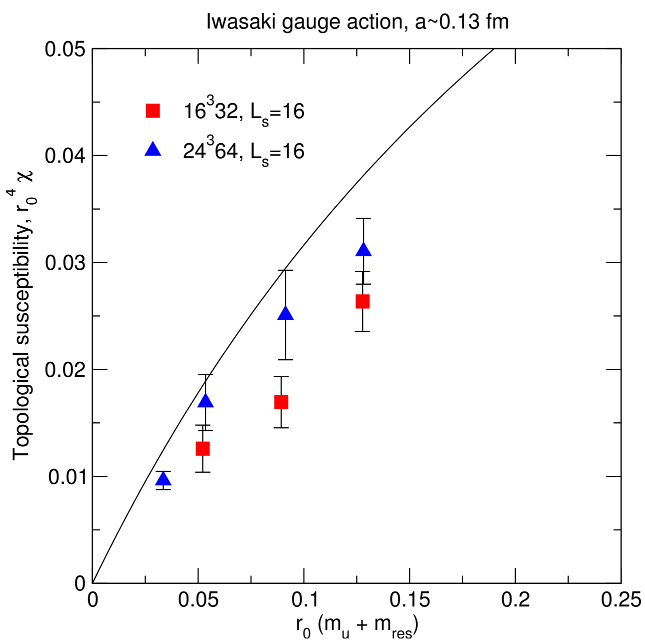
understand scaling

Topological susceptibility

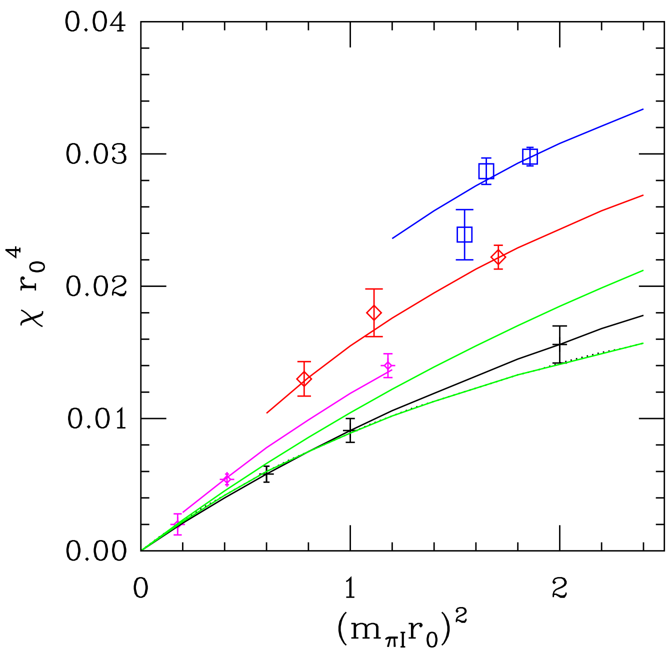
→ $\chi_{\rm topo}$ shows right behaviour in chiral limit

→ $\chi_{\rm topo}$ particularly important for fixed topology

(RBC-UKQCD)

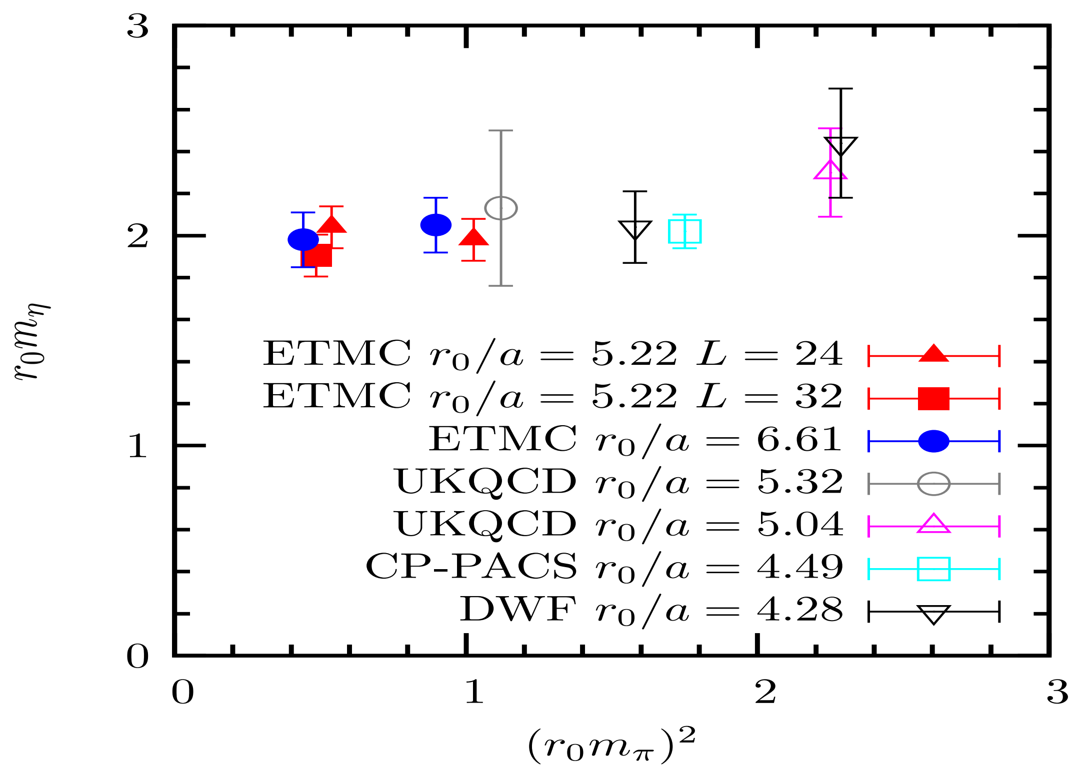


(MILC)



η_2 mass

- $\eta_2 \quad (N_f = 2)$ analogue of $\eta' \quad (N_f = 2+1)$



(ETMC)

$\longrightarrow$ reach small pion masses

$\longrightarrow$ confirm mass of $\eta_2 \approx 700$MeV

Finite size effects

Comparison of data at several volumes to :

rSχPT

	observed	"boosted"	1-loop rSχPT
quantity	$28^3 - 20^3$	$\infty - 20^3$	$\infty - 20^3$
af_π	1.4(2)%	1.6(2)%	1.1%
af_K	0.4(3) %	0.4(3) %	0.3%
$(am_\pi)^2$	−1.0(4)%	−1.2(4)%	−0.9%
$(am_K)^2$	−0.4(2)%	−0.4(2)%	−0.2%

(MILC)

$M_{\rm PS}L = 4$

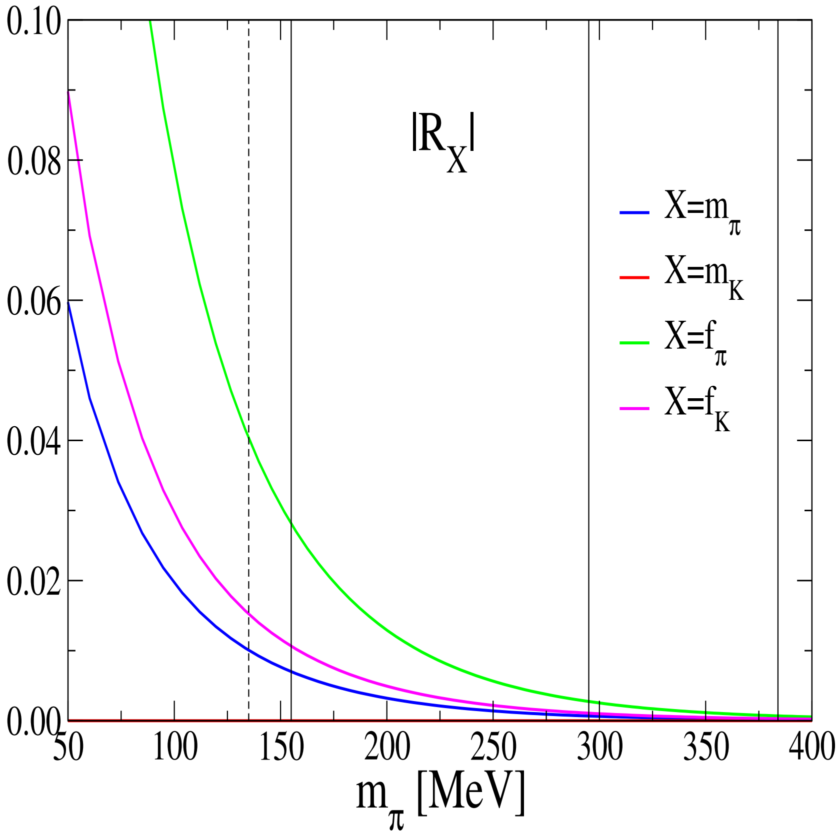
CDH (Colangelo, Dürr, Haefeli)

observ.	$M_{\rm PS}L$	meas. [%]	CDH [%]
$M_{\rm PS}$	3.0	+6.2	+6.1
$f_{\rm PS}$	3.0	−10.7	−10.3
$M_{\rm PS}$	3.5	+1.1	+1.5
$f_{\rm PS}$	3.5	−1.8	−2.9

(ETMC)

relative deviation: $R_O = \frac{O_L - O_\infty)}{O_\infty}$

Finite size effects from SU(3) ChPT

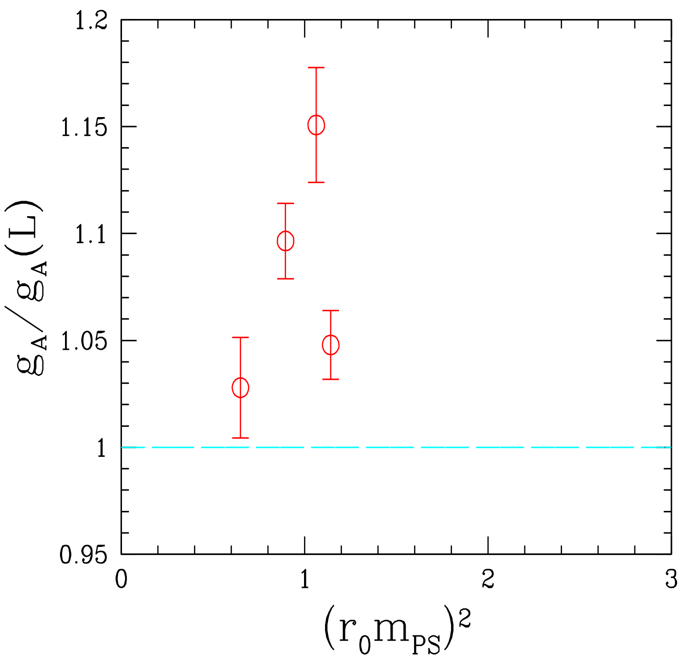


(PACS-CS)

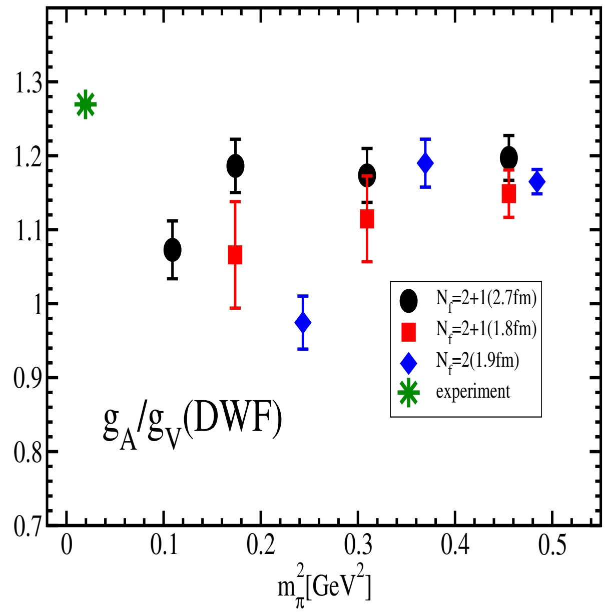
- $R_X = (X(L) - X(\infty))/X(\infty)$
- $L = 3\text{fm}$

$\longrightarrow$ finite size effects small even at physical point

Dangerous finite size effects



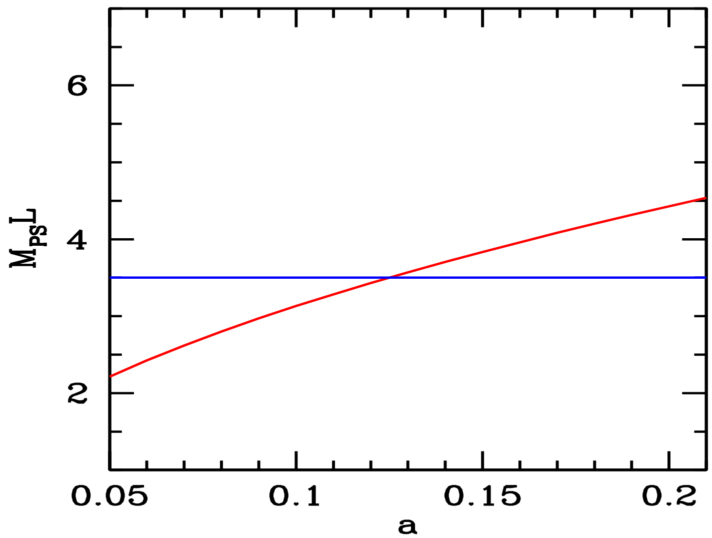
(QCDSF)

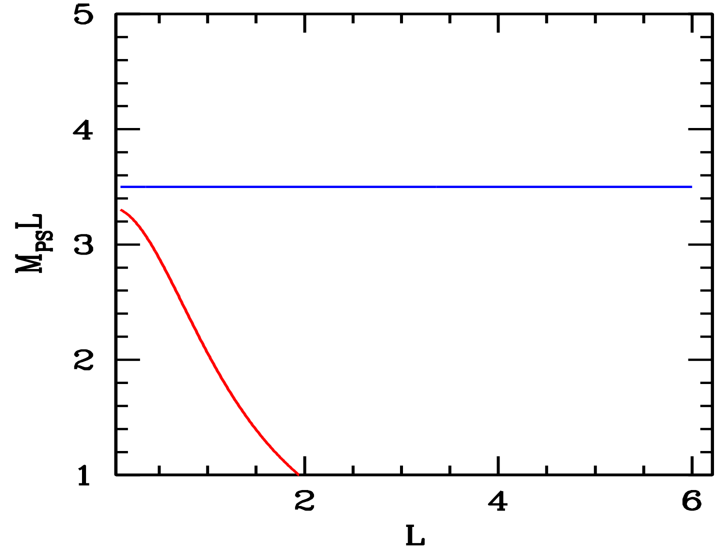


(RBC-UKCD)

predict: $L = 2.5$fm, $M_{\rm PS} = 140$MeV: 20%

Some bounds for simulations





stability bound

$$m_\pi L \geq \sqrt{3\sqrt{2}aB/Z}$$

δ expansion

finite size effects

$$M_{\rm PS}L \geq 3.5$$

minimal pion mass

$$M_{\rm PS}L \geq \frac{3/2 * f_0^2 L^2}{1. + 5.7/4 * \pi * f_0^2 L^2}$$

Getting social

- **ILDG:** put configurations on the net! **(talk by T. Yoshie)**

- **Codes:** publish code **(MILC (arXiv:0806.2312), Lüscher, Borici)**

- **Techniques:** publish papers with all technical details

Challenges for dynamical simulations

- Decay of unstable particles, resonances
- Disconnected contributions
- Change of topological charge towards the continuum limit
- Blind test of data analysis
- Collaborations with non-lattice people
  e.g.: (Allison et.al., arXiv:0805.2999)

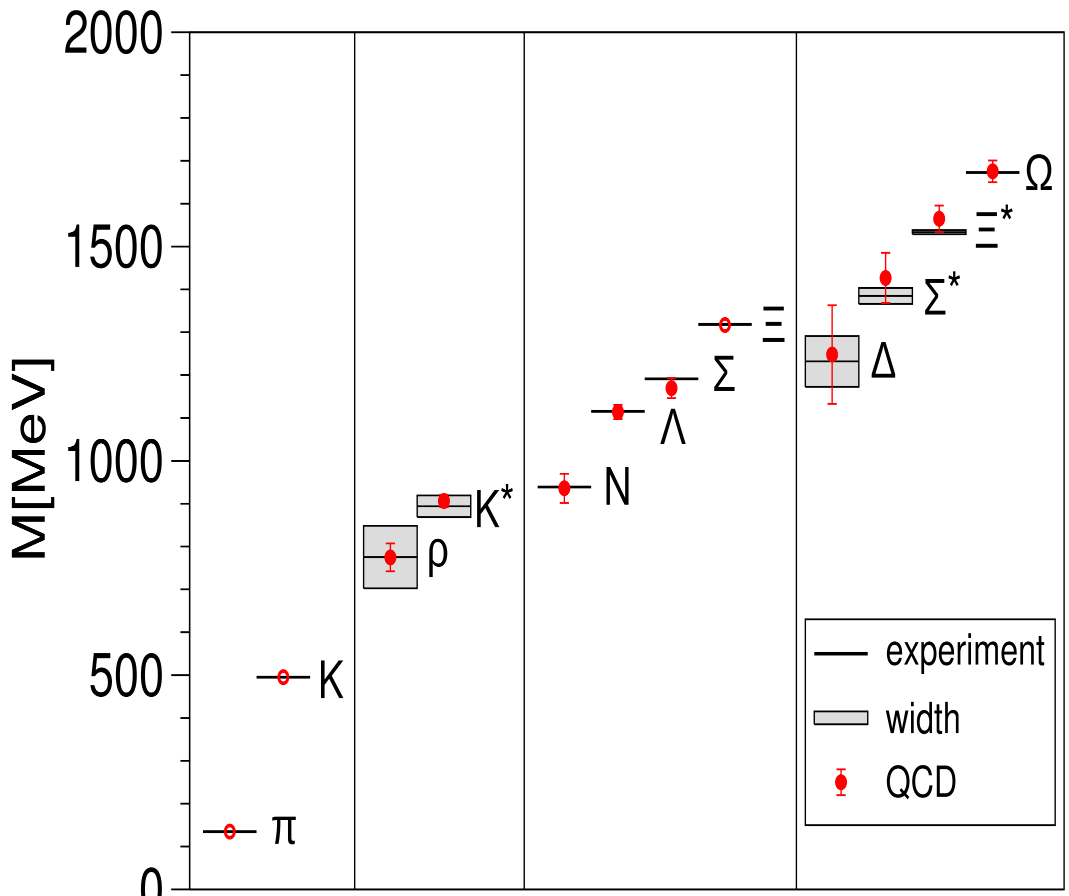
Conclusion: there is a rooting problem!

Who do we root for now?
Which dynasty do we want continuing to wave its victorious flag?

- thanks to algorithmic, machine and conceptual improvements:
  $\longrightarrow$ after many years of preparatory work simulations are done at
  - Pion mass: $200\mathrm{MeV} \lesssim M_{\mathrm{PS}}$ and even $M_{\mathrm{PS}} = 140\mathrm{MeV}$
  - lattice spacing: $0.05\mathrm{fm} \lesssim a$
  - lattice size: $M_{\mathrm{PS}} \cdot L \geq 3.5$
- investigate more: systematics of different lattice formulations:
  fourth root, stouting, isopin breaking, autocorrelations,
  residual mass, topology fixing, ...
- observations:
  - scaling towards continuum limit problematic, e.g. f_{PS}
  - applicability of χPT up to the strange quark questionable
  - need massless renormalization with dynamical strange quark
  - dangerous finite size effects, e.g. g_A
  - mixed action may have non-negligible cutoff effects

Conclusion: whom to root for?

- **the dynasties:**
  BMW, CLS, PACS-CS, ETMC, JLQCD, MILC, QCDSF, PACS-CS, RBC-UKQCD
  Let's go for all ⇒ universality will tell



(BMW collaboration)